Sebacic acid, isohexyl 4-isopropoxyphenyl ester

Inchi: InChI=1S/C25H40O5/c1-20(2)12-11-19-28-24(26)13-9-7-5-6-8-10-14-25(27)30-23-17-15

InchiKey: DWAMIJYOOCLZRG-UHFFFAOYSA-N

Formula: C25H40O5

SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1ccc(OC(C)C)cc1

Mol. weight [g/mol]: 420.58

Physical Properties

Property code	Value	Unit	Source
gf	-315.32	kJ/mol	Joback Method
hf	-966.65	kJ/mol	Joback Method
hfus	53.87	kJ/mol	Joback Method
hvap	94.13	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.479		Crippen Method
mcvol	360.100	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	2971.00		NIST Webbook
tb	977.18	K	Joback Method
tc	1196.35	K	Joback Method
tf	547.00	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1211.69	J/mol×K	977.18	Joback Method
cpg	1228.12	J/mol×K	1013.71	Joback Method
cpg	1242.90	J/mol×K	1050.24	Joback Method
cpg	1256.05	J/mol×K	1086.77	Joback Method
cpg	1267.60	J/mol×K	1123.29	Joback Method
cpg	1277.58	J/mol×K	1159.82	Joback Method
cpg	1286.02	J/mol×K	1196.35	Joback Method
dvisc	0.0002896	Pa×s	547.00	Joback Method
dvisc	0.0001356	Pa×s	618.70	Joback Method

dvisc	0.0000744	Pa×s	690.39	Joback Method
dvisc	0.0000456	Pa×s	762.09	Joback Method
dvisc	0.0000305	Pa×s	833.79	Joback Method
dvisc	0.0000217	Pa×s	905.48	Joback Method
dvisc	0.0000162	Pa×s	977.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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